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NEWS 2 AUG 06 CAS REGISTRY enhanced with new experimental property tags
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NEWS 4 AUG 13 CA/CAplus enhanced with additional kind codes for granted patents
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NEWS 6 AUG 27 Full-text patent databases enhanced with predefined patent family display formats from INPADOCDB
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NEWS 12 SEP 17 CA/CAplus enhanced with printed CA page images from 1967-1998
NEWS 13 SEP 17 CAplus coverage extended to include traditional medicine patents
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NEWS 15 OCT 02 CA/CAplus enhanced with pre-1907 records from Chemisches Zentralblatt
NEWS 16 OCT 19 BEILSTEIN updated with new compounds
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NEWS 22 DEC 17 USPATOLD added to additional database clusters
NEWS 23 DEC 17 IMSDRUGCONF removed from database clusters and STN
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NEWS 25 DEC 17 TOXCENTER enhanced with 2008 MeSH vocabulary in MEDLINE segment
NEWS 26 DEC 17 MEDLINE and LMEDLINE updated with 2008 MeSH vocabulary
NEWS 27 DEC 17 CA/CAplus enhanced with new custom IPC display formats
NEWS 28 DEC 17 STN Viewer enhanced with full-text patent content from USPATOLD
NEWS 29 JAN 02 STN pricing information for 2008 now available
NEWS 30 JAN 16 CAS patent coverage enhanced to include exemplified prophetic substances
NEWS 31 JAN 28 USPATFULL, USPAT2, and USPATOLD enhanced with new custom IPC display formats
NEWS 32 JAN 28 MARPAT searching enhanced
NEWS 33 JAN 28 USGENE now provides USPTO sequence data within 3 days of publication
NEWS 34 JAN 28 TOXCENTER enhanced with reloaded MEDLINE segment
NEWS 35 JAN 28 MEDLINE and LMEDLINE reloaded with enhancements

NEWS 36 FEB 08 STN Express, Version 8.3, now available

NEWS EXPRESS FEBRUARY 08 CURRENT WINDOWS VERSION IS V8.3,
AND CURRENT DISCOVER FILE IS DATED 24 JANUARY 2008

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STRUCTURE FILE UPDATES: 19 FEB 2008 HIGHEST RN 1004621-14-0
DICTIONARY FILE UPDATES: 19 FEB 2008 HIGHEST RN 1004621-14-0

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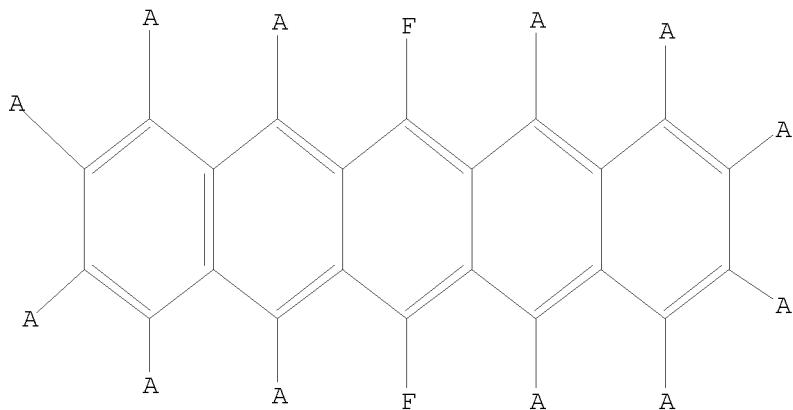
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L1 STRUCTURE UPLOADED

=> d 11
L1 HAS NO ANSWERS
L1 STR



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SAMPLE SEARCH INITIATED 09:29:59 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -      81 TO ITERATE

100.0% PROCESSED      81 ITERATIONS          0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE  **COMPLETE**
BATCH    **COMPLETE**

PROJECTED ITERATIONS:      1081 TO      2159
PROJECTED ANSWERS:          0 TO      0
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L2 0 SEA SSS SAM L1

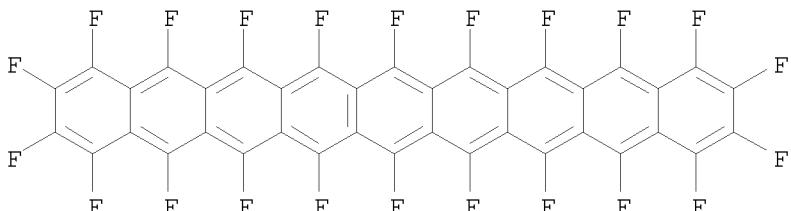
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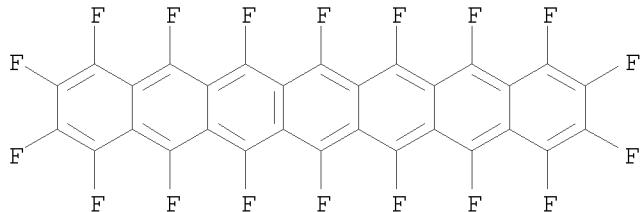
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L3      11 ANSWERS      REGISTRY      COPYRIGHT 2008 ACS on STN
IN      INDEX NAME NOT YET ASSIGNED
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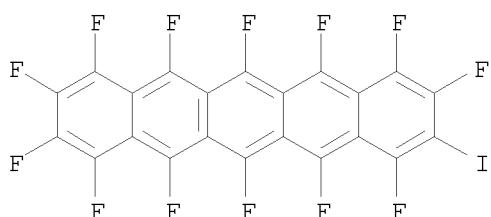
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):5

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MF C30 F18



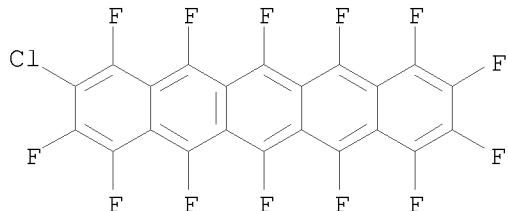
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 11 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN Pentacene, 1,2,3,4,5,6,7,8,9,11,12,13,14-tridecafluoro-10-iodo-
MF C22 F13 I



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

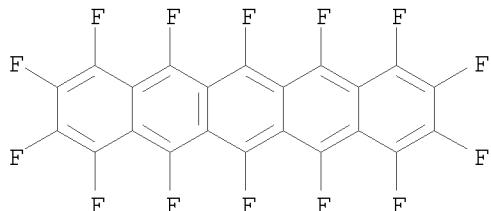
L3 11 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN Pentacene, 2-chloro-1,3,4,5,6,7,8,9,10,11,12,13,14-tridecafluoro-
MF C22 Cl1 F13



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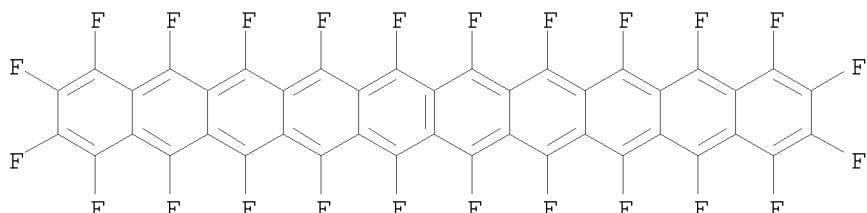
L3 11 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN

IN Pentacene, 1,2,3,4,5,6,7,8,9,10,11,12,13,14-tetradecafluoro-
MF C22 F14



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L3 11 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN INDEX NAME NOT YET ASSIGNED
MF C42 F24



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=> s 13
L4 19 L3

=> s 13 not py > 2003
19 L3
5355707 PY > 2003
L5 1 L3 NOT PY > 2003

=> s 13 not py > 2004
19 L3
4248038 PY > 2004
L6 4 L3 NOT PY > 2004

=> d 16 ibib abs hitstr 1-
YOU HAVE REQUESTED DATA FROM 4 ANSWERS - CONTINUE? Y/(N):y

L6 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2004:577543 CAPLUS
DOCUMENT NUMBER: 141:260225
TITLE: The essential role of H-F substitution in the
electron-phonon interactions and electron transfer in
the negatively charged acenes
AUTHOR(S): Kato, Takashi; Yamabe, Tokio
CORPORATE SOURCE: Fukui Institute for Fundamental Chemistry, Kyoto
University, Sakyo-ku, Kyoto, 606-8103, Japan
SOURCE: Journal of Chemical Physics (2004), 121(5), 2356-2366
CODEN: JCPSA6; ISSN: 0021-9606
PUBLISHER: American Institute of Physics
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The single charge transfer through acenes, partially H-F substituted
acenes, and fluoroacenes is discussed. The reorganization energies
between the neutral mols. and the corresponding monoanions for partially
H-F substituted acenes lie between those for acenes and fluoroacenes. The
delocalization of the lowest unoccupied MOs (LUMO) by substituting
hydrogen atoms by fluorine atoms with the highest electronegativity in
every element is the main reason why the reorganization energy between the
neutral mol. and the monoanion for partially H-F substituted acenes lies
between those for acenes and fluoroacenes. This result implies that the
neg. charged partially H-F substituted acenes would be better conductors
with rapid electron transfer than the neg. charged fluoroacenes if we
assume that the overlap of the LUMO between partially H-F substituted
acenes is not significantly different from that between two neighboring
fluoroacenes. The structures of the monoanions of acenes, fluoroacenes,
and partially H-F substituted acenes are optimized under D2h geometry, and
the Jahn-Teller effects in the monoanions of benzene and fluorobenzene are
discussed. The vibration effect onto the charge transfer problem is also
discussed. The C-C stretching modes around 1500 cm⁻¹ are the main modes
converting the neutral mols. to the monoanions in acenes, fluoroacenes,
and partially H-F substituted acenes. It can be confirmed from the
calculational results that the C-C stretching modes around 1500 cm⁻¹ the
most strongly couple to the LUMO in these mols. The main reason why the
total electron-phonon coupling consts. (1LUMO) for the monoanions of
acenes in which four outer hydrogen atoms are substituted by fluorine
atoms are larger than those for the monoanions of acenes in which several
inner hydrogen atoms are substituted by fluorine atoms is suggested. The

relationships between the electron transfer and the electron-phonon interactions are discussed. The plot of the reorganization energies against the 1LUMO values is found to be nearly linear. In view of these results, the relationships between the normal and superconducting states are briefly discussed.

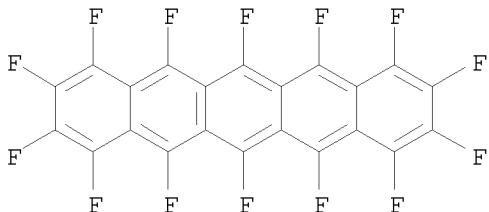
IT 646533-88-2 690975-12-3

RL: PRP (Properties)

(essential role of H-F substitution in electron-phonon interactions and electron transfer in neg. charged acenes)

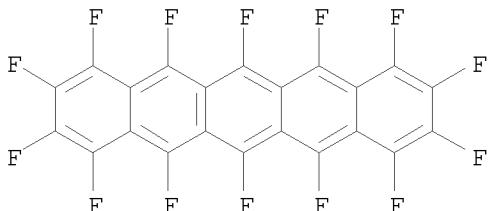
RN 646533-88-2 CAPLUS

CN Pentacene, 1,2,3,4,5,6,7,8,9,10,11,12,13,14-tetradecafluoro- (CA INDEX NAME)



RN 690975-12-3 CAPLUS

CN Pentacene, tetradecafluoro-, radical ion(1+) (9CI) (CA INDEX NAME)



REFERENCE COUNT: 99 THERE ARE 99 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:480070 CAPLUS

DOCUMENT NUMBER: 141:197895

TITLE: Perfluoropentacene: High-Performance p-n Junctions and Complementary Circuits with Pentacene

AUTHOR(S): Sakamoto, Youichi; Suzuki, Toshiyasu; Kobayashi, Masafumi; Gao, Yuan; Fukai, Yasushi; Inoue, Youji; Sato, Fumio; Tokito, Shizuo

CORPORATE SOURCE: Institute for Molecular Science, Okazaki, 444-8787, Japan

SOURCE: Journal of the American Chemical Society (2004), 126(26), 8138-8140

CODEN: JACSAT; ISSN: 0002-7863

PUBLISHER: American Chemical Society

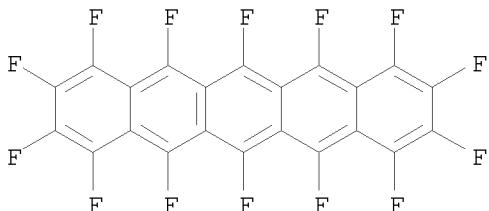
DOCUMENT TYPE: Journal

LANGUAGE: English

AB The authors report the synthesis and characterization of perfluoropentacene as an n-type semiconductor for organic field-effect transistors (OFETs). Perfluoropentacene is a planar and crystalline material that adopts a herringbone structure as observed for pentacene. OFETs with perfluoropentacene were constructed using top-contact geometry, and an electron mobility of 0.11 cm² V⁻¹ s⁻¹ was observed. Bipolar OFETs with

perfluoropentacene and pentacene function at both neg. and pos. gate voltages. The improved p-n junctions are probably due to the similar d-spacings of both acenes. Complementary inverter circuits were fabricated, and the transfer characteristics exhibit a sharp inversion of the output signal with a high-voltage gain.

IT 646533-88-2P, Perfluoropentacene
RL: DEV (Device component use); PNU (Preparation, unclassified); PREP (Preparation); USES (Uses)
(perfluoropentacene: high-performance p-n junctions and complementary circuits with pentacene)
RN 646533-88-2 CAPLUS
CN Pentacene, 1,2,3,4,5,6,7,8,9,10,11,12,13,14-tetradecafluoro- (CA INDEX NAME)



REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2004:297458 CAPLUS
DOCUMENT NUMBER: 140:429323
TITLE: Inverse isotope effects and electron-phonon coupling in the positively charged deutero- and fluoroacenes
AUTHOR(S): Kato, Takashi; Yamabe, Tokio
CORPORATE SOURCE: Fukui Institute for Fundamental Chemistry, Kyoto University, Sakyo-ku, Kyoto, 606-8103, Japan
SOURCE: Journal of Chemical Physics (2004), 120(16), 7659-7672
CODEN: JCPSA6; ISSN: 0021-9606
PUBLISHER: American Institute of Physics
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Electron-phonon interactions in the monocations of deutero- and fluoroacenes are studied and compared with those in the monocations of acenes and those in the monoanions of fluoroacenes. Because of the significant phase pattern difference between the highest occupied MOs (HOMO) and the lowest unoccupied MOs (LUMO), the frequency modes lower than 500 cm⁻¹ and the high-frequency modes around 1400 cm⁻¹ couple more strongly to the LUMO than to the HOMO, while the frequency modes around 500 cm⁻¹ and the frequency modes around 1600 cm⁻¹ couple more strongly to the HOMO than to the LUMO in fluoroacenes with D2h geometry. The total electron-phonon coupling consts. for the monocations (1HOMO) are estimated and compared with those for the monoanions (1LUMO) in deutero- and fluoroacenes. The 1HOMO values are estimated to be 0.418, 0.399, 0.301, 0.255, and 0.222 eV for C6F6 (1f), C10F8 (2f), C14F10 (3f), C18F12 (4f), and C22F14 (5f), resp. The 1HOMO values are smaller than the 1LUMO values in small fluoroacenes. But the 1HOMO value decreases with an increase in mol. size less rapidly than the 1LUMO value in fluoroacenes, and the 1HOMO value of 0.074 eV is much larger than the 1LUMO value of 0.009 eV in polyfluoroacene. The logarithmically averaged phonon frequencies for the monocations ($\omega_{ln, HOMO}$) are estimated to be larger than those for the monoanions ($\omega_{ln, LUMO}$) in fluoroacenes. This is because the C-C stretching modes around 1600 cm⁻¹ couple most strongly to the HOMO, and those around 1400 cm⁻¹ couple the most strongly to the LUMO in

fluoroacenes. The significant phase pattern difference between the HOMO and the LUMO is the main reason for the calculational results. The 1HOMO values increase much more significantly by H-F substitution than by H-D substitution in acenes. The possible inverse isotope effects in the electron-phonon interactions as a consequence of deuteration in the monocations of nanosized mols. are suggested.

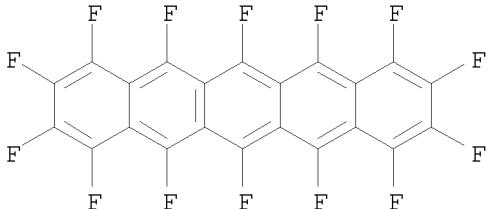
IT 690975-12-3

RL: PRP (Properties)

(inverse isotope effects and electron-phonon coupling in pos. charged deutero- and fluoroacenes)

RN 690975-12-3 CAPLUS

CN Pentacene, tetradeacafluoro-, radical ion(1+) (9CI) (CA INDEX NAME)



REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2003:898555 CAPLUS

DOCUMENT NUMBER: 140:118999

TITLE: Electron-phonon interactions in the monoanions of fluoroacenes

AUTHOR(S): Kato, Takashi; Yamabe, Tokio

CORPORATE SOURCE: Graduate School of Engineering, Department of Material Chemistry, Kyoto University, Sakyo-ku, Kyoto, 606-8501, Japan

SOURCE: Journal of Chemical Physics (2003), 119(21), 11318-11328

CODEN: JCPSA6; ISSN: 0021-9606

PUBLISHER: American Institute of Physics

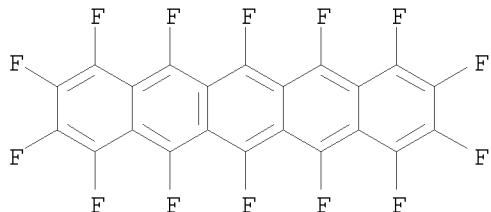
DOCUMENT TYPE: Journal

LANGUAGE: English

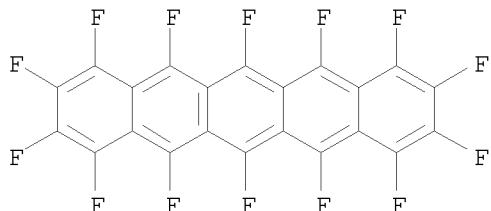
AB Electron-phonon interactions in the monoanions of fluoroacenes such as C₆F₆ (1f), C₁₀F₈ (2f), C₁₄F₁₀ (3f), C₁₈F₁₂ (4f), and C₂₂F₁₄ (5f) are studied, and compared with those in the monoanions of acenes and deutero-acenes. The C-C stretching modes around 1500 cm⁻¹ the most strongly couple to the lowest unoccupied MOs (LUMO) in fluoroacenes. The estimated total electron-phonon coupling consts. (1LUMO) are 0.475, 0.473, 0.350, 0.273, and 0.215 eV for 1f, 2f, 3f, 4f, and 5f, resp. The 1LUMO values for fluoroacenes are much larger than those for acenes and deuterio-acenes. Possible superconducting transition temps. (T_c) for the monoanions of deuterio-acenes and fluoroacenes are larger than those for the monoanions of acenes. The transition temperature (T_c) value increases much more significantly by H-F substitution than by H-D substitution in acenes. The 1LUMO and T_c values significantly decrease with an increase in mol. size from the monoanions of 1f to 5f. The logarithmically averaged phonon frequencies (ω_{ln}) do not significantly change with an increase in mol. size in the monoanions of fluoroacenes. The larger displacements of C atoms in the vibronic active modes in fluoroacenes than those in deuterio-acenes due to larger atomic mass of F than that of D, and the unchanged properties of the orbital patterns of the LUMO as a consequence of H-F and H-D substitution in acenes, are the main reasons why the 1LUMO value increases much more significantly by H-F substitution than by H-D

substitution, and the reason why the Tc value increases much more significantly by H-F substitution than by H-D substitution in acenes. The detailed properties of vibronic active modes and the electronic structures in the LUMO as well as the mol. wts. are closely related to the 1LUMO, ω_{ln} , and Tc values in the monoanions of fluoroacenes, deuteroacenes, and acenes.

IT 646533-88-2
RL: PRP (Properties)
(carbon-carbon bond lengths in)
RN 646533-88-2 CAPLUS
CN Pentacene, 1,2,3,4,5,6,7,8,9,10,11,12,13,14-tetradecafluoro- (CA INDEX NAME)



IT 645401-34-9
RL: PRP (Properties)
(electron-phonon interactions in)
RN 645401-34-9 CAPLUS
CN Pentacene, tetradecafluoro-, radical ion(1-) (9CI) (CA INDEX NAME)



REFERENCE COUNT: 90 THERE ARE 90 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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